The Extended UNIQUAC model for electrolyte solutions is an excess Gibbs energy function consisting of a Debye-Huckel term and a term corresponding to the UNIQUAC equation. For vapor-liquid equilibrium calculations, the fugacities of gas-phase components are calculated with the Soave-Redlich-Kwong equation of state. The model only requires binary, temperature-dependent interaction parameters. It has previously been used to describe the excess Gibbs energy for aqueous electrolyte mixtures and aqueous electrolyte systems containing methanol. It has been found to be an adequate model for representing solid-liquid-vapor equilibrium and thermal property data for strongly non-ideal systems. In this work, the model is extended to aqueous salt systems containing higher alcohols. The calculations are based on an extensive database consisting of salt solubility data, vapor liquid equilibrium data, and liquid-liquid equilibrium data for solvent mixtures and for mixed solvent-electrolyte systems.

The application of this model to represent the vapor-liquid-liquid-solid equilibria in aqueous systems containing various non-electrolytes (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl 1-propanol, 2-methyl 2-propanol) and various ions (Na+, K+, NH4+, Cl−, NO3, SO42−, SO32−, HSO3−, CO32−, and HCO3−) shows the capability of the model to accurately represent the phase behavior of these kinds of systems. (C) 2004 Elsevier Ltd. All rights reserved.